tert-Butyl alcohol 75-65-0 | DTXSID8020204

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Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 7.57 days

Global applicability domain: Inside

Local applicability domain index: 5.04e-01

Confidence level: 8.85e-01

Nearest Neighbors from the Training Set

Image not found

Pentane

Measured: 40.7 **Predicted:** 6.52

Image not found

n-Hexane

Measured: 157 Predicted: 7.45

Image not found

Octane

Measured: 157 Predicted: 8.57

Image not found

Nonane

Measured: 157 Predicted: 8.49 Image not found

Heptane

Measured: 88.3 Predicted: 7.54